Numerical Modelling of CO_2-Storage

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Introduction: Storage of CO_2 in the sub-surface is seen as a technology that can contribute to the generally accepted goal of a de-carbonized society. As real field experiments are hardly feasible, many current studies utilize the capabilities of numerical modelling.

Concerning the practical application of CO_2 storage many questions are still unanswered. In the most favoured scenario CO_2 in supercritical state is pressed into a deep geological formation. Within the permeable layer CO_2 will come to overlie brine and will start to dissolve into the deeper part by diffusion, which is influenced by convection.

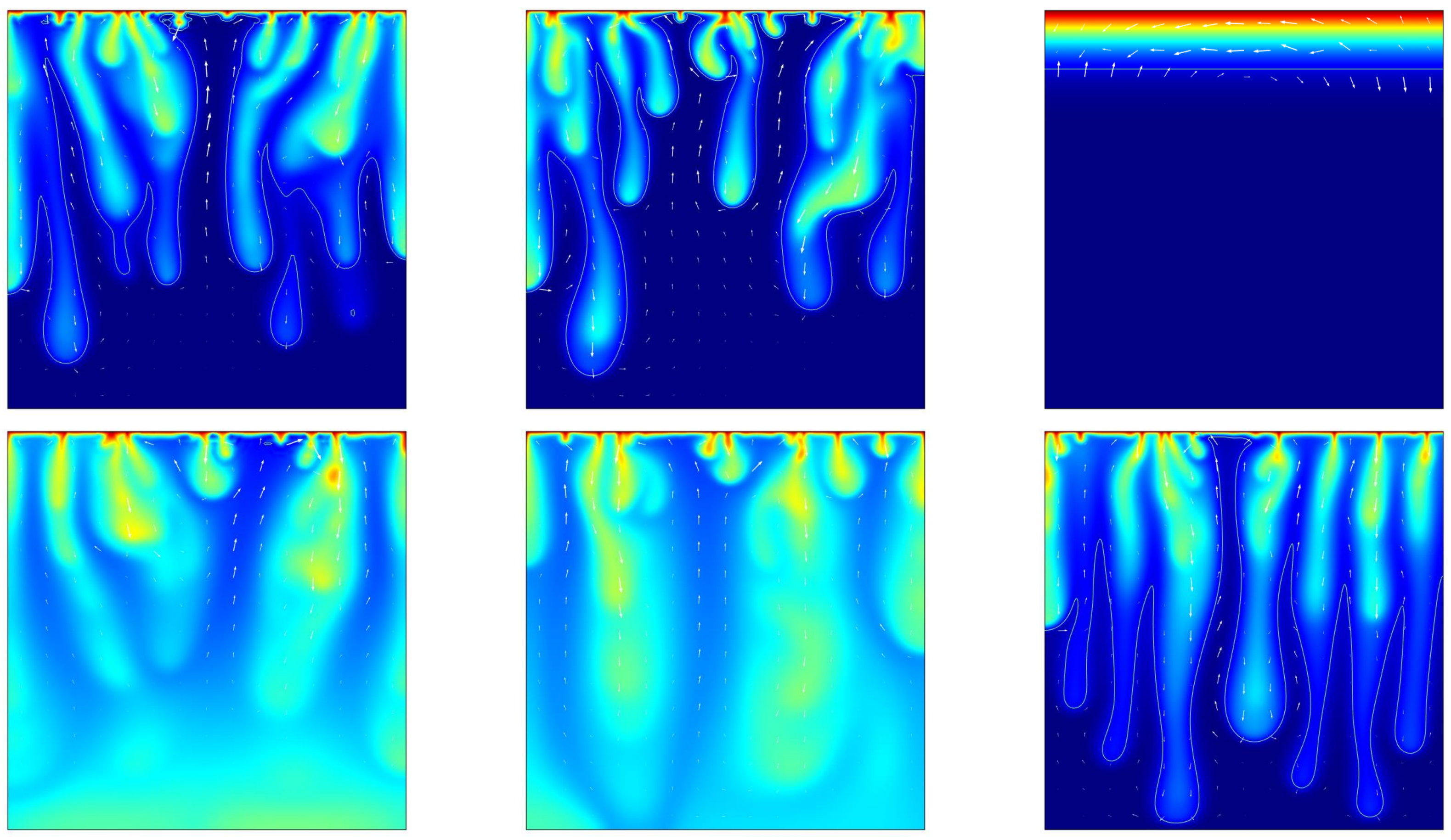

Figure 1. CO_2 concentration distributions (red: saturated, blue: zero; top: early convection, bottom: late convection; left: coarse mesh, center: medium mesh, right: fine mesh)

Convection is a multi-physics phenomenon, in which flow and transport processes are coupled. For the coupling the fluid density is the crucial parameter. For the highly dynamic processes of CO_2 storage, with high Rayleigh number, the initial phase with pure diffusion is followed by a convection phase. The latter can be sub-divided in an early stage with high but fluctuating mass transfer; and a late stage, in which mass transfer is decreasing[2].

Computational Methods: Flow and transport are described by a non-linear set of two partial differential equations: (1) one for the streamfunction Ψ, which includes the dimensionless Rayleigh number Ra, and (2) for the normalized concentration c[1,3]:

$$\frac{\partial}{\partial x}\left(\frac{\partial \Psi}{\partial x}\right)+\frac{\partial}{\partial z}\left(\frac{\partial \Psi}{\partial z}\right)=-Ra\frac{\partial c}{\partial x} \quad \text{with} \quad Ra=\frac{gk\Delta\rho H}{\mu D} \qquad (1)$$

$$\frac{\partial c}{\partial t}=\nabla\cdot(\nabla c-\mathbf{v}c) \quad \text{with} \quad v_x=-\frac{\partial \Psi}{\partial z} \quad \text{and} \quad v_z=\frac{\partial \Psi}{\partial x} \qquad (2)$$

The following sketch shows the 2D model region within a vertical cross-section through the formation and the boundary conditions:

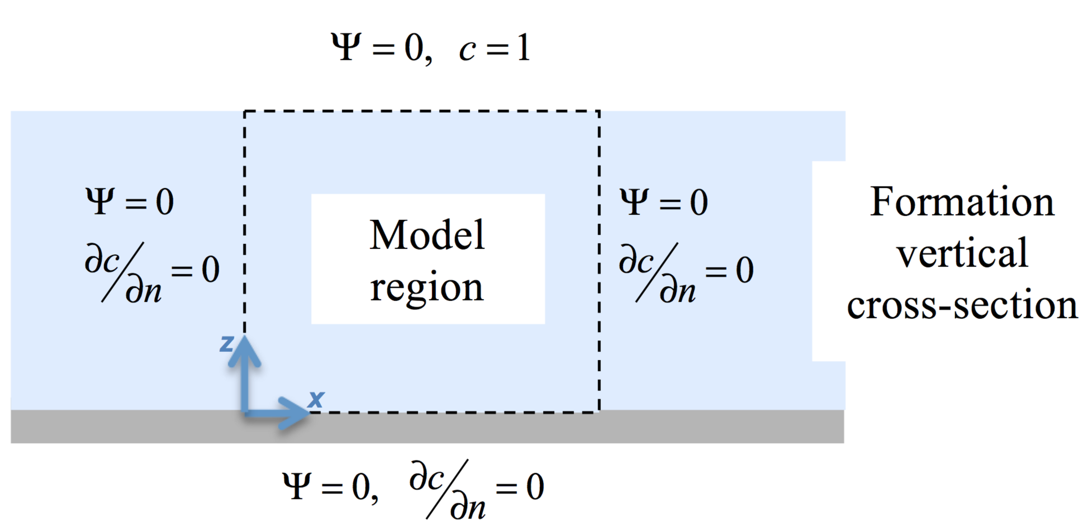

Figure 2. Model region & boundary conditions

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Results: Using COMSOL Multiphysics® the inhomogeneity of the permeability field, realized by random distributions were explored, as well as mesh dependencies. Input parameters are given in Table 1.

Parameter	Value [Unit]	Parameter	Value [Unit]
Saturated CO_2 mass fraction	0.0493	Density difference $\Delta\rho$	10.45 kg/m^3
Viscosity μ	$0.5947\bullet10^{-3}$ Pa•s	Molecular diffusivity D	$2\bullet10^{-9}$ m^2/s
Brine density	994.56 kg/m^3	Permeability k *(mean value)*	$5\bullet10^{-13}$ m^2

Table 1. List of reference case parameters[4]

The input Rayleigh number Ra was 5000. Fig. 3 shows the temporal development of mean mass transfer obtained from 10 realisations for 3 different meshes. The lower figure is obtained by shifting the fine mesh results in order to match the 'onset on convection' point.

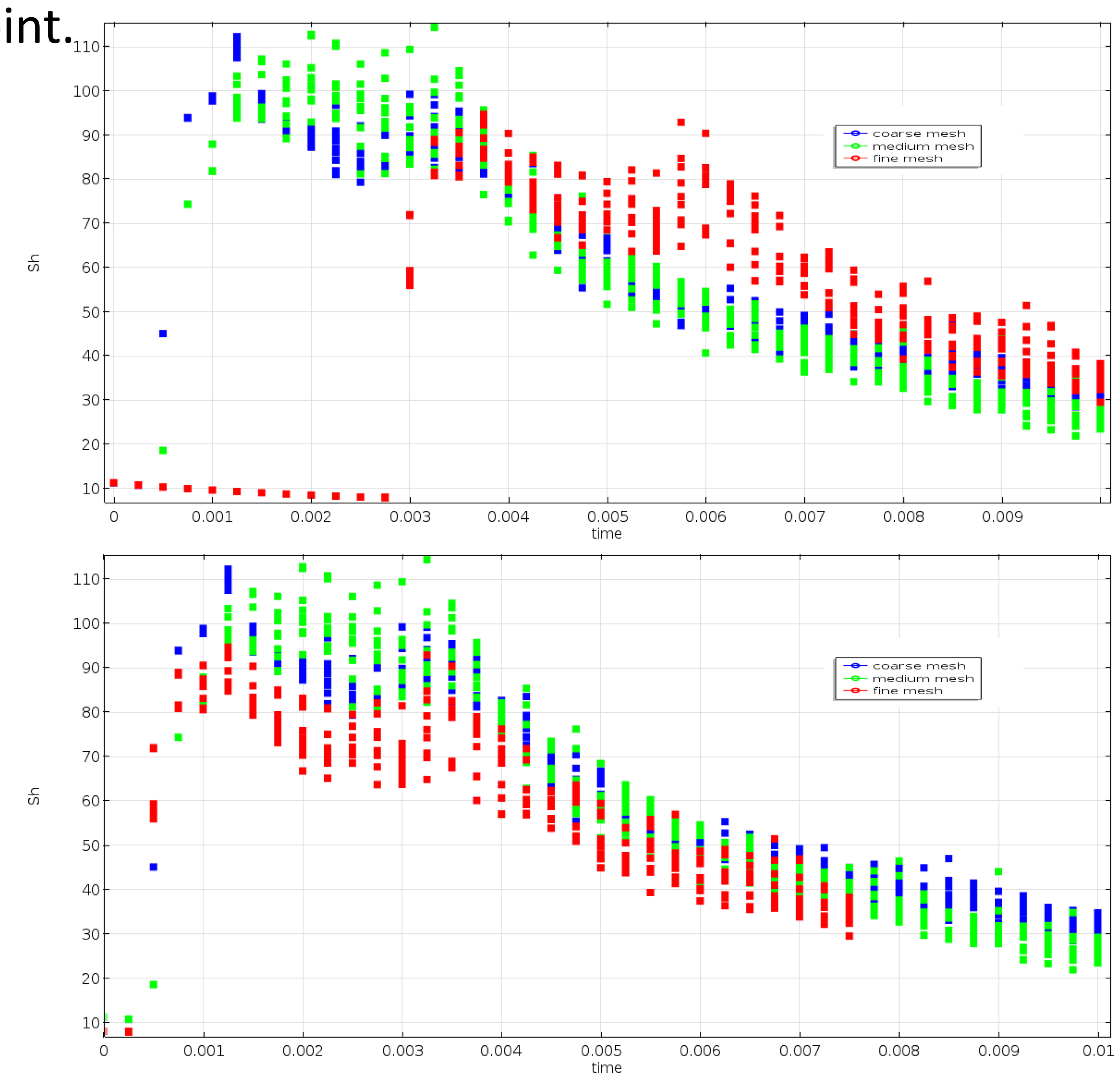

Figure 3. Mass transfer range, indicated by the Sherwood number Sh for 30 different scenarios

Conclusions: The details of the flow patterns depend heavily on disturbances of physical parameters and on numerical features. Comparing mass transfer of 30 scenarios, a range for mass transfer during the different stages is obtained. Despite the differences in the single scenarios the duration of the early convection stage turns out to be a constant. Moreover, in the late convection stage the range of fluctuations is decreasing.

References:

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